Cross Section Evaluation Working Group

Summary of the CSEWG Meeting on ENDF/B-VII Validation

Oak Ridge National Laboratory
July 13, 2005

Participants

More than 20 people attended the meeting. M. Chadwick, LANL and P. Oblozinsky, BNL chaired the meeting.

Agenda

1) Opening remarks (P. Oblozinsky)
2) Overview comments (M. Chadwick) Link 1
3) Preliminary ENDF/B-VII (M. Herman) Link 2, 3
   - Status, data verification
   - Deficiencies: Zr isotopes, 237-Np, Pa isotopes, other
4) Individual file improvements
   - 9-Be (LANL) Link 4, 5, 6
   - 232-Th (LANL)
   - S(alpha, beta) issues (LANL) Link 7, 8, 9
   - Fission products (P. Oblozinsky) Link 10
   - Actinide photonuclear (LANL)
   - Other files: Am isotopes, 51-V, other Link 11
5) Assessment of alternate sets of files Link 12, 13, 14
   - 235-U (thermal nubar)
   - 1-H
6) Validation results Link 15, 16, 17, 18
   - Actinides
   - Other
7) Covariances
   - Gd (L. Leal, T. Kawano, M. Herman)
   - Re and 233-U (L. Leal)
   - Standards
   - Processing
8) Timetable for ENDF/B-VII release

Overview comments

Chadwick reviewed the progress achieved since November 2004 CSEWG meeting.

Preliminary ENDF/B-VII

Herman reviewed the status of beta0 release, explained data verification done by the NNDC and discussed deficiencies known to the NNDC.

Individual File Improvements: Action Item List - See Bold Items!

1. Gd-156, 158, 160 will be redone by **Leal in the resonance region. 155 and 157 will be improved by BNL and LANL**. New versions with only cross sections (without covariances) will be released in September for the Beta-1 library.

2. 242,242mAm and 243,245Cm had no fission neutrons**. Talou/Young/Kawano will check these files – we think the Am files are already fixed.**

3. Ca-00 crashes in HEATR. **MacFarlane will check.**

4. New LANL 89Y, 191,193Ir, and Tm-169 dosimetry files could be made complete evaluations and put into. **Do by the B-VII release if possible- Herman.**

5. 237Np. Existing LANL file is reasonable. No action.

6. Cu-63, 65. Russ complains about performance**. Kawano will ask JENDL about their file.**

7. 232Th. Replace by JEFF/Maslov or IAEA/Herman/Leal. **Action – Herman.**

8. List of problems found by Herman, eg NJOY/RESEND calc. –ve cross sections, residual nucleus incorrect, nonzero threshold, etc. Herman will post this list. Prompt KE of gammas = 6 eV (instead of MeV). Many of these have been cleaned and fixed by Dunford. The current status of these problems should be re-assessed for B-VII, and then fixed! **Herman will generate updated list of problems; Little/ MacFarlane/Kawano will try to fix, and will distribute this list.**

9. 238Np and some others end at a very low energy. Should these be thrown out for B-VII – or subsitute using other JENDL evaluations? **Action: Kawano /Little/Herman.**

10. Cullen reported problems with files: Mg24, Ar40, K-41, Ti istopes, Ni-59, and 238Np, Cf-253,Es-253, we'll consider taking them from JEFF/ JENDL. (Other materials he listed, such as 3,4He, 6Li, natC are fine we think – eg the n2n threshold is above 20 MeV, so not a problem). **Then we would eliminate the Ti-nat evaluation, etc. Look into adoption JEFF evaluations for the dosimetry files. Herman will do this (and other natural v. isotopic evaluation issues). Blair Briggs will look into Ti benchmarks.**

11. Zr isotopes. **Herman suggests a possible adopting the SG21 recommendations**, which involve mixtures of new BNL, JENDL, and BROND. Blair notes HEU-COMP-INTER-005 and COM-MIXED-003 Obninsk Zr criticality assembly this will test Zr. **Cecil and Skip will test. BNL will send SG23 recommended files immediately and Cecil and Skip will test, together with the JENDL files. Kawano will also check these as he has studied capture for these. Cecil will give an assessment by early Sep 2005.**

12. Pa-231, 232, 233. We should ask Trkov's opinion on which are the best files. **LANL/Chadwick should also look at the Bordeaux/ Geel fission data. Assess whether or not to take 2 isotopes from JENDL (for 231,233)**

13. 232Th. ENDF is old but does have covariances. There is a new IAEA/CRP file from Leal (resolved), unresolved (Geel), and Herman. This needs to be tested – after Leal has finished his work. We can test high energy performance against THOR. Mosteller's light-water breeder test can be done too. Leal can make covariance data with IAEA high-energy estimates too.

14. Mosteller – likes many aspects of the new evaluations, but…UNRES res region for 235U. ZEUS assembly (HEU plates with graphite with Cu reflector). As the spectrum changes, there's a big trend in B-VI and B-VII evaluations – softer spectrum leads to a drop in reactivity, whereas B-V is better. Is this due to 235U unresolved resonance range? **This poor performance is in contrast to HEU_MET_FAST-7 results from Kahler, where things looked good. We'll discuss with Mosteller, but no changes likely before beta-1.**

15. Mosteller - Th: The original ENDF performs poorly, Maslov/JEFF performes better; Mosteller – SB-5 (which includes U and Th, in thermal) shows 0.9957 (low). But we're not sure why- the JEFF Th doesn't much improve this. IEU-COMP-INTER-ICI-001 has 4 cases with 40-49% absorption in Th, from fast – thermal. Current results for thermal are badly off (7-8% off!). **Leal/Herman to finalize a Th232 for testing by MacF and Mosteller, with the additional Th benchmark ICI-001 involving testing. Leal to give LANL by August 1, 2005.**

16. Fast cross sections for Cu: Unmoderated ZEUS benchmark (HEU with Cu reflector). We now calc 1% high for new B-VII. B-VI looks better. Look into how JENDL Cu performs. (JEFF used ENDF6.8 Cu). BTW, Comet uses a Cu reflector, so it would be good to have it right – McKnight notes we should check that the integral assembly model is right. **Kawano will look at JENDL Cu data, and Bob/Russ already has processed and will test.**

17. Mosteller: 233U – 2 thermal cases he looked at, one has k above and one below 1, so hard to assess new thermal nubar 0.3 % change.

18. Mosteller: 239Pu thermal Pu-ST-09 calculates 2% high. This is one of many experiments , and there are trends that many have noted (eg Heinrich). Can't be solved by B-VII. No action.

19. 1D angular distributions. VI.4 to VI.8 led to poor performance with the new 2H angular distributions, in reflected HEU spheres. But another series of unreflected cylinders with large error bars that perform better with new data. Hale is also looking at microscopic predictions. **Hale will study this with a recommendation for beta-1 in September 2005.**

20. 233U – check Heinrich's previous testing to assess the 0,3% possible change for nubar-thermal. **Dave Heinrich will dig up old data testing results and distribute, and then use beta-0 files to recalc, along with the modified thermal value. Bob will send Dave the ACE files.**

21. 9Be. The new result – using Hale's R-matrix analysis for the total elastic, looks much better – the Be thickness bias is much reduced. Westfall suggests looking at some benchmarks that have Be. Need to also check the LANL Pu/HEU –with Be reflectors. ZIPR-20 cores are massively over-predicted, and need to be calculated too (space reactor criticals). Ber ball is in progress**. LANL/Hale will also explore using Hale's angular distributions too. We will use the new Hale version of 9Be – and explore using Hale's angular distributions.**

22. S-alpha-beta. MacFarlane studied the methods used. MCNP works at 293.6K, but ENDF has data at 296K. MacFarlane recomputed S at 293.6, for better self-consistency. Also, there were too few grid points on the alpha-beta grid in the evaluation, and putting in more points improved the results based on the integrals. The number of incident energies was also changed. MCNP sampling scheme was also changed to use an improved sampling.

    Overall conclusions MacFarlane's new result for water is very similar to Mattes's; the thermal assemblies, with best continuous MCNP, to up very slightly. Can also run with the old un-patched MCNP, with just slightly higher results. MacFarlane results for HST42 using the new S-alpha-beta (and the 332.6 mb H capture) give very good results, very close to the European values. Mattes has additional sources of temperature-dependence, compared to the ENDF model. MacFarlane needs to check the temperature dependences – Hogenberg pointed to one potential problem. Mattes' model for water shows improved agreement with microscopic data but both Mattes and MacFarlane/GA results look equally good in criticality applications. For heavy water, Mattes' results show significant improvements. She used an ability to include coherent effects. Conclusions – use Mattes for heavy water. Decide between Mattes and MacFarlane for light water in the coming weeks, and decide by Sep 2005 for beta-1 release. For U and U-O, MacFarlane's fixed evaluations can be used. MacFarlane needs to modify the one(s) submitted to BNL. Also, he has an Al metal and Fe evaluation – should also be submitted.

    Bob will give us recommendations and files by Sep 2005. Bob will also supply Cecil with total cross section, with temperature dependence.

23. 1H. MacFarlane – going from 332.0mb to the Standard value of 332.6mb, causes about 0.1 – 0.06% decreases in k-eff. (but, note that the temp effects would take it down slightly. There were arguments presented by Lubitz and Kahler that they preferred the 332.0 value. They would see a drop by 0.14%. Our tentative conclusion is to stick with 332.0mb – it is within the experimental error bar (332.6+- 0.7). **MacFarlane et al will test** Hale's new latest-latest 1H evaluation and **Hale will**

discuss with Carlson whether this should be the one used in the standards (this still has 332.0 at thermal).

24. Skip Kahler. Used RCP01 calculations, using B/VI.8 and VII.beta0. Overall: k=1.00000(14)-0.0023(50)*A A=above fraction leakage. Pretty good. He then looked at faster assemblies, HUE-MET-FAST-007 from ORNL – the B-VII data look much better – they are hotter, and k is v. close to 1. HEU metal with polyethylene – at various spectrum hardnesses everything looks much better. No trend in calculations for the 26 assemblies. Generally, Bettis codes are 0.1% lower than MCNP. Using the Mattes kernel instead of ENDF results in a very tiny decrease in k – in the noise. MacFarlane saw a tiny increase. LCT-6 look excellent - 1.000 essentially.

25. 208Pb. Skip saw some effects of poor Pb reflection for LCT10.1-4 (they over-calculate), and we noted that we need to assess 206. 207Pb too. There are also indications that LCT10.9-13 for iron reflectors also shows too much over-calculation**. Kawano will look at improving scattering in Pb isotopes**.

26. **Bob will send Cecil and Dick all s-alpha-beta kernels for BeO/BE O Be/O kernels**.

27. All natural evaluations will be removed from b1 if isotopic evaluations are available. **Action BNL**.

28. Fission products. SG23 prepared and revised 164 files, 29 files are currently reviewed by BNL-KAERI, remaining 25 files should be completed shortly. **Most of these 218 files will be available for b1, action Oblozinsky**.

29. Fission products. Deficiencies in URR noted by K. Guber on 155,157Gd (will give information to BNL), **Y. Danon will provide his new data to BNL** (data not yet published).

30. Fission products. **NJOY99 patch for JENDL-3.3 should be used by NJOY2003 – MacFarlane**.

31. Photonuclear. LANL is working on improved photonuclear data for actinides, current Obninsky files will be replaced by new LANL. **LANL will supply new actinide files for b1.**

32. 51-V. BNL made a modification, too high H production at 14 MeV (complaint from fusion community). BNL fixed the problem. **Improved file will be included in b1.**

Validation Results

33. McFarlane reported b0 Actinides testing.

- U235 spectrum too soft, inelastic scattering probably?
- 233U pretty good
- Bigten consistent with Godiva

- McFarlane will look into U235 spectrum (?) and some other issues, small changes only.

34. Lubitz: Thermal 235U standards, what to do? Fission agrees (new, VI.5, old standard), scattering cross section differ quite a lot, little can be done to change this. Nubar: old-new = -0.14%, k1 new 721.606, old 719.49, nubar can be adjusted, the only option. Lubitz suggested to ignore 235U thermal nubar from standards. Nubar already higher in JEFF-3.1 compared to new standards. **We need next round of standards, then repeat the exercise and decide what to do.**

Covariances

35. Gd. **Action BNL, ORNL, LANL**: Resonances 156,158, 160Gd from BNL to ORNL; fast region 155, 157Gd new from BNL to LANL. New covariances will be produced by ORNL and LANL. It remains open what to do with 156, 158, 160Gd fast.

36. Re. Ok, in future new resonance data from RPI. No action.

37. 233-U. Resonance region is ok. Kawano will discuss with Mark what to do with fast region.

38. 232-Th. Leal will provide covariances for resonances in RRR and URR (August 2005). Fast region is feasible, will be done later (BNL, LANL).

39. 235,238U and 239 Pu covariances will be done probably in 2006. No action.

40. Covariances for standards. **Action**: LANL will provide 11-B evaluation (end of July 2005?). Then, Pronayev will need 2 months to produce covariances for single materials. Full covariance matrix is not needed.

41. Processing. ORNL will have something operational this fall (M. Dunn). NJOY – no plan for this year, McFarlane wants to process MF=30 for hydrogen. ERRORJ, author Chiba, some improvements underway, not his main job, may invite him to LANL. NNDC should use NJOY and ERRORJ from Leal to process new covariances for b1.

42. Bob Little: What to do with covariances from B-VI.8? **Bob should provide recommendation on this.**

Some main conclusions

Stick with our beta0 1H, 235nu values for now. Cecil would like even hotter, but standards say softer. We need to sort out differences between codes before we can make changes.

Timetable for ENDF/B-VII Release

September beta1, November CSEWG meeting, release December 2005.